Puromycin

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 326 °C

Global applicability domain: Outside

Local applicability domain index: 6.54e-02

Confidence level: 6.31e-01

Nearest Neighbors from the Training Set

Image not found
Ametryn
Measured: 345
Predicted: 341

Image not found
Desmetryn
Measured: 345
Predicted: 341

Image not found
2,4,6-Tricyano-1,3,5-triazine
Measured: 262
Predicted: 264

Image not found
Auramine
Measured: 331
Predicted: 349

Image not found
Tetraethylenepentamine
Measured: 342
Predicted: 339